Quantization of Hyperbolic N-Sphere Scattering Systems in Three Dimensions

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Abstract

Most discussions of chaotic scattering systems are devoted to two-dimensional systems. It is of considerable interest to extend these studies to the, in general, more realistic case of three dimensions. In this context, it is conceptually important to investigate the quality of semiclassical methods as a function of the dimensionality. As a model system, we choose various three dimensional generalizations of the famous three disk problem which played a central role in the study of chaotic scattering in two dimensions. We present a quantum-mechanical treatment of the hyperbolic scattering of a point particle off a finite number of non-overlapping and non-touching hard spheres in three dimensions. We derive expressions for the scattering matrix **S** and its determinant. The determinant of **S** decomposes into two parts, the first one contains the product of the determinants of the individual one-sphere **S**-matrices and the second one is given by a ratio involving the determinants of a characteristic KKR-type matrix and its conjugate. We justify our approach by showing that all formal manipulations in these derivations are correct and that all the determinants involved which are of infinite dimension exist. Moreover, for all complex wave numbers, we conjecture a direct link between the quantum-mechanical and semiclassical descriptions: The semiclassical limit of the cumulant expansion of the KKR-type matrix is given by the Gutzwiller-Voros zeta function plus diffractional corrections in the curvature expansion. This connection is direct since it is not based on any kind of subtraction scheme involving bounded reference systems. We present numerically computed resonances and compare them with the corresponding data for the similar two-dimensional N-disk systems and with semiclassical calculations.

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1 Introduction

Many if not most of the concepts in quantum chaos were developed and are being applied to two-dimensional systems. This is due to the relative simplicity of those systems as compared to three-dimensional ones. To find the periodic orbits in a generically three-dimensional geometry, obviously requires much more work than performing the same type of analysis in a two-dimensional billiard, say. However, since the real world is three-dimensional, an extension of chaos studies to more realistic systems is called for. The celebrated Hydrogen Atom in a strong magnetic field can be reduced to an, effectively, two dimensional system due to the cylindrical symmetry of the problem. Similar simplifications also exist in other systems. Recently, a full-fledged study of the three-dimensional Sinai-billiard has been performed [1]. Here, we present a study of a chaotic scattering system in three dimensions. We investigate several generalizations of the two-dimensional three disk problem. We chose three-dimensional versions of this system since it played an important role in the development of many concepts and methods in chaotic scattering. In order to describe N-sphere scattering systems quantum-mechanically we extend the methods of Refs. [2, 3] to three dimensions. A related approach was already used in Ref. [4] to describe the multiple scattering of an electron in non-overlapping muffin-tin potentials. In Ref. [5] the scattering of a point particle on non-symmetric configurations of point-scatterers in three dimensions was investigated.

In general, hyperbolic or even chaotic *scattering* systems have some advantages compared with *bounded* systems, if one is interested in the quantum-mechanical *and* the semiclassical description of a classically chaotic problem. Chaotic bounded systems are normally plagued by the presence of non-isolated, non-hyperbolic bouncing ball orbits (see, e.g., the Sinai-billiard or the stadium billiard), the importance of very long periodic orbits, and the problem that without fine-tuning a la Berry and Keating [6] the semiclassical Gutzwiller-Voros zeta function [7, 8] would not predict *real-valued* energy eigenvalues. In contrast, the geometry of hyperbolic scattering systems can easily be chosen such that bouncing ball orbits are absent. Furthermore, the contributions of longer periodic orbits to the scattering matrix are automatically suppressed relatively to the shorter ones and no fine-tuning is necessary in order to predict scattering resonances as they are anyhow complex-valued.

Two-dimensional N-disk and three-dimensional N-sphere systems are examples of such scattering systems which are simple enough to be studied *in all detail* semiclassically and quantum-mechanically. In the past the two-dimensional Sinai-billiard, which can be interpreted as the scattering on an infinite, regular array of equal disks, has been quantized [9] using the Korringa-Kohn-Rostoker (KKR) method [10]. More recently the scattering of a point particle on hard disks in two dimensions [11] has been studied classically [12, 13], quantum-mechanically [2, 3] and semiclassically [14, 15, 16, 17] using the techniques of periodic orbit theory [7]. The range of validity of the purely geometrical semiclassical input has been investigated in Refs. [18, 19]. In Refs.[20, 21, 22] $\hbar$-corrections to the geometrical periodic orbits were constructed, whereas the authors of Refs.[23, 24, 25] extended the Gutzwiller-Voros zeta function to include diffractive creeping periodic orbits as well. Recently a formalism which also includes the limit of small disks ($ka \ll 1$, k: wave number, a: radius of the disk) was presented [26]. In Ref. [3] the connection between the quantum-mechanical and semiclassical descriptions of N-disk scattering systems has been investigated in detail. On the

experimental side, the scattering on two equal disks was investigated using microwave cavities [27]. In Ref. [28] the two-dimensional Sinai-billiard was treated in a scattering approach and in Ref. [29] diffractive effects were considered.

Here we focus on the analogous scattering systems of N spheres in three dimensions. These systems are still simple enough to be treated quantum-mechanically, semiclassically and classically. The quantum-mechanical description of N-sphere systems is similar to the two-dimensional N-disk case, as essentially the same approach can be used. Also the semiclassical description with purely geometrical input is similar to the two-dimensional case. But diffractional corrections should be substantially different as the corresponding creeping orbits are now extrema on two-dimensional manifolds instead of one-dimensional ones. A detailed quantum-mechanical description of N-sphere scattering systems is presented and the connection with the semiclassical treatment is investigated.

The paper is organized as follows. In Sec. 2, we derive an explicit expression for the scattering matrix within the framework of stationary scattering theory using Green's theorem. We do this in some detail to make the paper self-contained. In Sec. 3, the determinant of the scattering matrix is re-written as a product of an incoherent part and a coherent part. We show that the scattering resonances are given by the zeros of a KKR-type matrix. Moreover, we conjecture a direct link between the quantum mechanical and semiclassical descriptions of N-sphere systems involving the Gutzwiller-Voros zeta function plus diffractional corrections. This connection is valid for all complex wave numbers. In Sec. 4, we give a proof that all formal manipulations performed in the preceding sections are allowed and that the determinants of the infinite matrices involved are well defined. In Sec. 5, we present numerical results on two-, three- and four-sphere scattering systems and compare them with the analogous two- and three-disk systems. In Sec. 6, we summarize our results and give an outlook.

2 Calculation of the Scattering Matrix

We describe the scattering of a point particle on N hard spheres within the framework of stationary scattering theory following the methods of Berry [9] and Gaspard and Rice [2]. In Sec. 2.1, we define the scattering matrix and outline our approach. In Sec. 2.2, the elements of the scattering matrix are worked out explicitly.

2.1 Definitions and General Concepts

To describe a generic configuration of N spheres we use the following notation: $j \in \{1, \ldots, N\}$ specifies one spherical scatterer with radius a_j. $R_{jj'}$ denotes the distance between the centers of the spheres j and j'. To specify positions we use $N+1$ coordinate systems: First we choose a global coordinate system (x, y, z) whose origin is situated at an arbitrary point in the neighbourhood of the N scatterers. This point is chosen to be the center of the large sphere of the integration volume used in Green's theorem (see Sec. 2.2). If the scattering configuration possesses symmetries the origin of the global system is placed at the symmetry center of the entire system. In order to perform symmetry reductions we introduce N local coordinate systems, $(x^{(j)}, y^{(j)}, z^{(j)})$, whose origins lie at the centers of the N spheres. The axes of these coordinate systems are chosen in such a way that the symmetry of the entire

configuration is respected. The vector from the origin of the global coordinate system to the center of the j-th sphere is called $\vec{s}_j$ and it is measured in the global system. All the vectors in the local coordinate system of sphere j are measured relative to this vector. $\hat{R}^{(j)}_{jj'} \equiv \vec{R}^{(j)}_{jj'}/R_{jj'}$ denotes the unit vector from the center of the sphere j to that of j' and it is measured in the (j)-system. In general, vectors with an upper index (j) are measured in the (j)-system, vectors without upper index are measured in the global system.

A solution of the time-independent Schrödinger equation fulfills

$$\begin{aligned} \left(\vec{\nabla}^2 + \vec{k}^2\right)\psi(\vec{r}) &= 0\,, \quad \vec{r} \text{ outside the } N \text{ spheres,} \\ \psi(\vec{r}) &= 0\,, \quad \vec{r} \text{ on the surfaces of the spheres.} \end{aligned} \tag{1}$$

The energy of the particle is $\hbar^2\vec{k}^2/2m$ and $\vec{k}$ is the wave vector of the incident wave. We expand the wave function $\psi(\vec{r})$ in a basis of eigenfunctions of angular momentum

$$\psi(\vec{r}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} \psi^k_{lm}(\vec{r}) Y^*_{lm}(\hat{k}) \tag{2}$$

where k and $\hat{k}$ are the length and the solid angle of the wave vector, respectively. Because of this expansion, we construct solutions of the Schrödinger equation for the basis functions

$$(\vec{\nabla}^2 + \vec{k}^2)\psi^k_{lm}(\vec{r}) = 0\,. \tag{3}$$

Asymptotically for large distances from the scatterers ($kr \to \infty$) the spherical components ψ^k_{lm} can be written as a superposition of in-coming and out-going spherical waves,

$$\begin{aligned} \psi^k_{lm}(\vec{r}) \quad &\sim \quad \frac{2\pi}{kr}\sum_{l'=0}^{\infty}\sum_{m'=-l'}^{l'} \{ i^{l'} [e^{-i(kr - \frac{l+1}{2}\pi)} \delta_{ll'}\delta_{mm'} \\ &\qquad + \mathbf{S}_{lm,l'm'} e^{i(kr - \frac{l+1}{2}\pi)}] Y_{l'm'}(\hat{r}) \}\ . \end{aligned} \tag{4}$$

This equation defines the scattering matrix $\mathbf{S}$. Its elements $\mathbf{S}_{lm,l'm'}$ describes the scattering of an in-coming wave with angular momentum l, m into an out-going wave with angular momentum l', m'. If there are no scatterers, we have $\mathbf{S} = \mathbf{1}$ and the asymptotic expression of a plane wave $e^{i\vec{k}\cdot\vec{r}}$ is recovered. As is well known, the scattering matrix $\mathbf{S}$ is unitary because of probability conservation.

To derive an explicit expression for the $\mathbf{S}$-matrix, we use the free Green's function,

$$(\vec{\nabla}^2 + \vec{k}^2)G(\vec{r},\vec{r}\,') = -4\pi\delta^3(\vec{r}-\vec{r}\,') \quad , \quad G(\vec{r},\vec{r}\,') = G(\vec{r}\,',\vec{r}) \tag{5}$$

$$G(\vec{r},\vec{r}\,') = 4\pi i k \sum_{l=0}^{\infty}\sum_{m=-l}^{l} j_l(kr_<)\, h^{(1)}_l(kr_>)\, Y^*_{lm}(\hat{r}) Y_{lm}(\hat{r}\,')\ , \tag{6}$$

where $r_<$ ($r_>$) denotes the magnitude of the shorter (longer) of the two vectors $\vec{r}$ and $\vec{r}\,'$ whose directions can be expressed in any coordinate system. The Green's function and the components $\psi^k_{lm}(\vec{r})$ of the wave function are inserted in Green's theorem which yields

$$\begin{aligned}
\int_V d^3r \, \Big[\psi^k_{lm}(\vec{r})\,(\vec{\nabla}^2 + \vec{k}^2)G(\vec{r},\vec{r}\,') - G(\vec{r},\vec{r}\,')\,(\vec{\nabla}^2 + \vec{k}^2)\psi^k_{lm}(\vec{r})\Big] \\
= -4\pi \int_V d^3r \, \psi^k_{lm}(\vec{r})\delta^3(\vec{r} - \vec{r}\,') \\
= \int_{\partial V} d\vec{a} \cdot \Big[\psi^k_{lm}(\vec{a})\vec{\nabla}G(\vec{a},\vec{r}\,') - G(\vec{a},\vec{r}\,')\vec{\nabla}\psi^k_{lm}(\vec{a})\Big] \\
= \begin{cases} 0 & \vec{r}\,' \notin V, \\ -4\pi\psi^k_{lm}(\vec{r}\,') & \vec{r}\,' \in V, \end{cases}
\end{aligned} \tag{7}$$

where V denotes the integration volume and ∂V is its boundary. The appropriate volume of integration V consists of a large sphere centered at an arbitrary point in the neighbourhood of the N scatterers. Its radius is chosen to be so large that asymptotic formulae like Eq. (4) hold for points far away from the origin but still inside the integration volume. From this large sphere we exclude N spheres whose centers coincide with those of the N scatterers and whose radii are larger by an infinitesimal amount ϵ than the corresponding radii of the scatterers.

2.2 Computation of the Matrix Elements

Equation (7), understood in the limit $\epsilon \to 0$, can now be applied to two different cases as we can choose the point $\vec{r}\,'$ to be outside or inside the volume V. In the first case $\vec{r}\,'$ is chosen to be some point on the surface of the scatterer j and therefore outside the integration volume V. In the second case $\vec{r}\,'$ is chosen to lie inside the volume V and its modulus r' is taken to be so large that asymptotic formulae like Eq. (4) hold. The boundary ∂V decomposes into $N{+}1$ disjoint parts: The outer boundary of the large sphere, $\partial_\infty V$, and the N surfaces $\partial_j V$ of the excluded spheres, which coincide with the scatterers in the limit $\epsilon \to 0$.

First case: $\vec{r}\,' \equiv \vec{r}_j \in$ boundary of the $j^{\,\text{th}}$ scatterer
All components ψ^k_{lm} vanish on the surfaces of the scatterers, but the gradient of the wave function on these surfaces is nonzero. Its normal component can be expanded in spherical harmonics, $Y_{lm}(\hat{r}^{(j)}_j)$, defined on the surface of the $j^{\,\text{th}}$ scatterer,

$$\vec{n}_j \cdot \vec{\nabla}\psi^k_{lm}(\vec{r}_j) \equiv \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{l'} \mathbf{A}^j_{lm,l'm'} Y_{l'm'}(\hat{r}^{(j)}_j) \tag{8}$$

where $\vec{n}_j$ denotes a unit vector perpendicular to ∂V pointing outside V. The orientation $\hat{r}^{(j)}_j$ is measured in the (j)-system. The unknown coefficients $\mathbf{A}^j_{lm,l'm'}$ are then uniquely determined through Green's theorem (7). In this way the gradient of the wave function is characterized by the matrix $\mathbf{A}^j$ which depends on the sphere label j and whose matrix elements are specified by angular momentum quantum numbers. Collecting everything, we

arrive at a compact matrix formulation which expresses the gradient matrix $\mathbf{A}$ in terms of two matrices $\mathbf{C}$ and $\mathbf{M}$

$$\mathbf{C}^j = \mathbf{A}^{j'} \cdot \mathbf{M}^{j'j} \; . \tag{9}$$

where we use the Einstein-summation convention for the sphere indices j and j'. The matrix elements of $\mathbf{C}^j$ and $\mathbf{M}^{jj'}$ read

$$\begin{aligned}
\mathbf{C}^j_{lm,l'm'} &= \frac{(4\pi)^{\frac{3}{2}}}{ika_j^2} \sum_{l_1=0}^{\infty} \sum_{\tilde{m}=-l'}^{l'} (-1)^m \, i^{l_1+l'} \\
&\quad \times \sqrt{(2l+1)(2l_1+1)(2l'+1)} \begin{pmatrix} l_1 & l' & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l' & l \\ m-\tilde{m} & \tilde{m} & -m \end{pmatrix} \\
&\quad \times \frac{j_{l_1}(ks_j)}{h^{(1)}_{l'}(ka_j)} Y_{l_1,m-\tilde{m}}(\hat{s}_j) D^{l'}_{m'\tilde{m}}(gl,j)
\end{aligned} \tag{10}$$

and

$$\begin{aligned}
\mathbf{M}^{jj'}_{lm,l'm'} &= \delta^{jj'} \delta_{ll'} \delta_{mm'} \\
&\quad + (1-\delta^{jj'}) \left(\frac{a_j}{a_{j'}} \right)^2 \sqrt{4\pi} (-1)^m \sum_{l_1=0}^{\infty} \sum_{\tilde{m}=-l'}^{l'} i^{l_1+l'-l} \\
&\quad \times \sqrt{(2l+1)(2l_1+1)(2l'+1)} \begin{pmatrix} l_1 & l' & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l' & l \\ m-\tilde{m} & \tilde{m} & -m \end{pmatrix} \\
&\quad \times j_l(ka_j) \frac{h^{(1)}_{l_1}(kR_{jj'})}{h^{(1)}_{l'}(ka_{j'})} Y_{l_1,m-\tilde{m}}(\hat{R}^{(j)}_{jj'}) D^{l'}_{m'\tilde{m}}(j,j') \; .
\end{aligned} \tag{11}$$

Details are given in App. A. Here, $j_l(z)$ and $h^{(1)}_l(z)$ are spherical Bessel functions and Hankel functions of first kind, respectively [30]. The vectors $\vec{s}_j$ are measured in the global coordinate system attached to the large sphere of integration and point from its origin to the center of the $j^{\,\text{th}}$ sphere (which is of radius a_j), s_j is its modulus, and $\hat{s}_j$ the corresponding unit vector. $\vec{R}_{jj'}$ is the vector from the center of the sphere j to the center of j' as measured in the local coordinate system attached to the $j^{\,\text{th}}$ sphere, $R_{jj'}$ is its modulus and $\hat{R}_{jj'}$ the corresponding unit vector. $D^l_{m,m'}(gl,j')$ and $D^l_{m,m'}(j,j')$ are the rotational matrices which transform the local coordinate system of sphere j' to the global coordinate system and to the local coordinate system of sphere j, respectively. Finally, we use the definition of Ref. [31] for the $3j$-symbols.

Second case: $\vec{r}\,' \in V$, r' large

Because of Green's theorem (7) we have an explicit expression for $\psi^k_{lm}(\vec{r})$ which yields inserted into the asymptotic expansion (4) an explicit formula for the scattering matrix

$$\mathbf{S} = \mathbf{1} - i\mathbf{A}^j \cdot \mathbf{D}^j \; , \tag{12}$$

where the elements of the matrix $\mathbf{D}^j$ are found to be

$$\begin{aligned}
\mathbf{D}^j_{lm,l'm'} &= \frac{ka_j^2}{\sqrt{\pi}} \sum_{l_1=0}^{\infty} \sum_{\tilde{m}=-l}^{l} (-1)^{\tilde{m}+l_1} i^{l_1-l} \\
&\quad \times \sqrt{(2l+1)(2l'+1)(2l_1+1)} \begin{pmatrix} l' & l_1 & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l' & l_1 & l \\ m' & \tilde{m}-m' & -\tilde{m} \end{pmatrix} \\
&\quad \times j_l(ka_j) j_{l_1}(ks_j) D^l_{\tilde{m}m}(j,gl) Y_{l_1,\tilde{m}-m'}(\hat{s}_j)\ .
\end{aligned} \tag{13}$$

Again, details are given in App. A. Here, the rotational matrix $D^l_{mm'}(j,gl)$ transforms the global coordinate system into the local coordinate system of the $j^{\text{ th}}$ sphere. The gradient matrix $\mathbf{A}^j$ appears again because of the boundary integrals on the scatterer surfaces.

Hence, combining the results of both cases, we can use Eq. (9) to eliminate the matrix $\mathbf{A}^j$ from Eq. (12) [2]. We finally arrive at

$$\mathbf{S} = \mathbf{1} - i\mathbf{C}^j \cdot \left(\mathbf{M}^{-1}\right)^{jj'} \cdot \mathbf{D}^{j'} \tag{14}$$

which is expressed in the global coordinate system. In order to shorten the notation we will suppress the labels j and j', unless otherwise specified.

As mentioned above the effects of the scattering on the N spheres are described by the product $-i\mathbf{C} \cdot \mathbf{M}^{-1} \cdot \mathbf{D}$ which is of course the on-shell $\mathbf{T}$-matrix. Examining the obtained formulae we see that $\mathbf{M}$ depends only on the relative positions of the scatterers and that it contains all the information about the geometry of the entire scattering system. It does not depend on the choice of the center of the large sphere in the integration volume and on the orientation of the corresponding global coordinate system. For these reasons we call $\mathbf{M}$ a characteristic matrix. It is of KKR-type [9, 10]. In contrast, the matrices $\mathbf{C}$ and $\mathbf{D}$ depend on this choice and furthermore do not contain any information about the relative positions of the N scatterers. We may therefore conclude that the coherent multi-sphere part of the scattering is contained in $\mathbf{M}$ while the single sphere aspects are contained in $\mathbf{C}$ and $\mathbf{D}$.

If one would like to construct $\mathbf{S}$ explicitly from Eq. (14), it would be necessary to find the inverse of the infinite matrix $\mathbf{M}$, which is a nontrivial task. But if one is only interested in spectral properties like scattering resonances it suffices to look for the poles of the determinant of the $\mathbf{S}$-matrix [4, 32, 33, 34]. The latter can be expressed in such a way that it does not involve $\mathbf{M}^{-1}$ any more (see the following Section). From Eq. (14) we expect that the resonances of the coherent part of the scattering are given by the zeros of the determinant of $\mathbf{M}$.

Before focussing on the determinant of $\mathbf{S}$, we should have a closer look at Eq. (9) which is only determined up to a transformation of the form $\mathbf{C'} \equiv \mathbf{CE} = \mathbf{AME} \equiv \mathbf{AM'}$. To get an unambiguous definition, we have chosen such a normalization that in the case of the scattering from only one sphere we have simply $\mathbf{C} = \mathbf{A}$. This choice implies $\mathbf{M} = \mathbf{1} + \mathbf{W}$ where the diagonal entries of $\mathbf{W}$ vanish. In Sec. 4 we sketch how to prove that $\mathrm{Tr}\,\mathbf{W}$ converges absolutely in every basis so that the determinant of $\mathbf{M}$ is well defined [35]. This is very important as $\mathrm{Det}\,\mathbf{M}$ plays a crucial role in calculating scattering resonances, as we will see now.

3 Determinant of the Scattering Matrix and the Link to the Semiclassical Zeta-Function

Since we are interested in the scattering resonances it is sufficient to find the poles of the determinant, det $\mathbf{S}$, of the scattering matrix [4, 32, 33, 34] as a function of complex wave number k. Obviously $\mathbf{S}$ is an infinite matrix, hence it is a nontrivial task to prove the existence of its determinant. To keep the discussion transparent, we postpone the formal proof to Sec. 4 and anticipate the mathematical soundness of the calculations to be performed. We work out an explicit expression for det $\mathbf{S}$ in Sec. 3.1. In Sec. 3.2, we conjecture a direct link to the semiclassical zeta-function.

3.1 Calculation of the Determinant

A formal definition of the determinant of an infinite matrix $\mathbf{Q} \equiv \mathbf{1} + \mathbf{P}$ is given by

$$\det(\mathbf{1}+\mathbf{P}) = \exp\{\mathrm{tr}\,[\ln(\mathbf{1}+\mathbf{P})]\}\ , \tag{15}$$

$$\ln(\mathbf{1}+\mathbf{P}) = -\sum_{n=1}^{\infty} \frac{(-1)^n}{n}\mathbf{P}^n\ . \tag{16}$$

Equation (15), understood as Taylor-expanded expression (i.e., in the cumulant expansion, see below), is well defined if tr $\mathbf{P}$ converges absolutely in every basis [35]. Formally one gets the following expression for the determinant of the N-sphere $\mathbf{S}$-matrix, $\mathbf{S}^{(N)}$,

$$\begin{aligned}
\det \mathbf{S}^{(N)} &= \exp\{\mathrm{tr}\ \ln(\mathbf{1} - i\mathbf{C}\cdot\mathbf{M}^{-1}\cdot\mathbf{D})\} \\
&= \exp\left\{-\sum_{n=1}^{\infty}\frac{i^n}{n}\mathrm{tr}\,[(\mathbf{C}\cdot\mathbf{M}^{-1}\cdot\mathbf{D})^n]\right\} \\
&= \exp\left\{-\sum_{n}\frac{i^n}{n}\mathrm{Tr}\,[(\mathbf{M}^{-1}\cdot\mathbf{D}\cdot\mathbf{C})^n]\right\} \\
&= \exp\{\mathrm{Tr}\ \ln(\mathbf{1} - i\mathbf{M}^{-1}\cdot\mathbf{D}\cdot\mathbf{C})\} \\
&= \mathrm{Det}\,(\mathbf{1} - i\mathbf{M}^{-1}\cdot\mathbf{D}\cdot\mathbf{C}) \\
&= \mathrm{Det}\,[\mathbf{M}^{-1}\cdot(\mathbf{M} - i\mathbf{D}\cdot\mathbf{C})] \\
&= \frac{\mathrm{Det}\,(\mathbf{M} - i\mathbf{D}\cdot\mathbf{C})}{\mathrm{Det}\,(\mathbf{M})}\ .
\end{aligned} \tag{17}$$

Here, we introduced capital case traces and determinants Tr $\cdots$ and Det $\cdots$ in order to indicate that they refer to matrices labeled by the index triples j, l, m, whereas the lower case traces and determinants act on matrices which are just labeled by the (angular momentum) index pairs l, m.

With the caveat that there might be also poles and zeros in the *numerator*, the resonances can be determined by just looking for the zeros of $\mathrm{Det}\,\mathbf{M}$ in the complex k-plane. In order to get a simpler expression for $\det \mathbf{S}^{(N)}$, which also gives more physical insight, we calculate the determinant of $\mathbf{X} \equiv \mathbf{M} - i\mathbf{D}\cdot\mathbf{C}$. With the knowledge of Eqs. (10) and (13) one can calculate the product $\mathbf{D}\cdot\mathbf{C}$. In order to do this, the properties of consecutive rotations (changes of coordinate systems) and the re-coupling of angular momenta via 6-j-symbols (see Ref. [31] for the necessary formulae) have to be considered. Here only the result will be given,

$$\begin{aligned}
\mathbf{D}^{j}_{lm,l''m''}\mathbf{C}^{j'}_{l''m'',l'm'} &= \frac{2}{i}\frac{j_l(ka_j)}{h^{(1)}_l(ka_j)}\delta^{jj'}\delta_{ll'}\delta_{mm'} \\
&\quad + (1-\delta^{jj'})\sum_{l_1=0}^{\infty}\sum_{M=-l'}^{l'}\left(\frac{a_j}{a_{j'}}\right)^2 \frac{2}{i}\sqrt{4\pi}\, i^{l_1+l'-l}(-1)^m \\
&\quad \times \sqrt{(2l+1)(2l'+1)(2l_1+1)}\,\frac{j_l(ka_j)}{h^{(1)}_{l'}(ka_{j'})} j_{l_1}(kR_{jj'})Y_{l_1,m-M}(\hat{R}^{(j)}_{jj'}) \\
&\quad \times \begin{pmatrix} l' & l & l_1 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l' & l & l_1 \\ M & -m & m-M \end{pmatrix} D^{l'}_{m'M}(j,j')\,. \qquad (18)
\end{aligned}$$

It is easy to see that the matrix $\mathbf{X} \equiv \mathbf{M} - i\mathbf{D}\cdot\mathbf{C}$ is given by

$$\mathbf{X}^{jj'}_{lm,l'm'} = (-1)^{m'-m}\mathbf{S}^{(1)}_{lm,l'm'}(j')\left(\mathbf{M}^{jj'}_{l,-m,l',-m'}\right)^* \,, \qquad (19)$$

where $\mathbf{M}^*$ is a shorthand for $(\mathbf{M}(k^*))^*$ and $\mathbf{S}^{(1)}(j;k)$ denotes the 1-scatterer $\mathbf{S}$-matrix for the scattering from a single sphere with radius a_j, described in a coordinate system whose origin lies in the center of the sphere,

$$\mathbf{S}^{(1)}_{lm,l'm'}(j') = -\frac{h^{(2)}_{l'}(ka_{j'})}{h^{(1)}_{l'}(ka_{j'})}\delta_{ll'}\delta_{mm'}\,. \qquad (20)$$

The last equation is easily obtained by a comparison of the exact solution of this integrable problem and the ansatz (4). The corresponding determinant, $\det \mathbf{S}^{(1)}(j;k)$, is of course independent of the coordinate system. We now have a (formal expression for the) product-structure for the determinant of $\mathbf{X}$,

$$\mathrm{Det}\,\mathbf{X}(k) = \mathrm{Det}\,(\mathbf{M}(k^*))^\dagger\left(\prod_{j=1}^{N}\det \mathbf{S}^{(1)}(j;k)\right)\,. \qquad (21)$$

Combining (21) and (17), we finally obtain

$$\det \mathbf{S}^{(N)}(k) = \frac{\mathrm{Det}\,(\mathbf{M}(k^*))^\dagger}{\mathrm{Det}\,\mathbf{M}(k)}\left(\prod_{j=1}^{N}\det \mathbf{S}^{(1)}(j;k)\right)\,. \qquad (22)$$

The determinant splits up into an incoherent part, consisting of the product of the N determinants of the one-scatterer $\mathbf{S}$-matrices, and a coherent part, given by the ratio of the

determinants of the hermitian conjugate of the characteristic matrix and the determinant of $\mathbf{M}$ itself. Equation (22) obviously respects the unitarity of the $\mathbf{S}$-matrix, as the one-scatterer $\mathbf{S}$-matrices (20) are by themselves unitary because of $(h_m^{(1)}(ka))^* = h_m^{(2)}(k^*a)$ and as the coherent part of $\det \mathbf{S}^{(N)}$ is manifestly unitary. As mentioned, the scattering resonances are given by the zeros of $\mathrm{Det}\,\mathbf{M}$. However, this determinant does not only possess zeros but also poles. These poles cancel the resonance poles of the incoherent part of $\det \mathbf{S}^{(N)}$, as $\mathrm{Det}\,\mathbf{M}$ and the product of the $\det \mathbf{S}^{(1)}$ both involve the same number and power of Hankel functions $h_l^{(1)}(ka_j)$. The same is true for the poles of $\mathrm{Det}\,\mathbf{M}^\dagger$ and the zeros of the product of the $\det \mathbf{S}^{(1)}$: both involve the same number and power of Hankel functions $h_l^{(2)}(ka_j)$.

It is clear that $\det \mathbf{S}^{(N)}$ does not depend on the choice of the global coordinate system that was used in the definition of the $\mathbf{S}$-matrix (4) and to fix the center of the large spherical integration volume in Green's theorem (7). As we are interested in the coherent part of the scattering we will deal with $\mathrm{Det}\,\mathbf{M}(k)$ from now on.

The symmetry of the scattering configuration leads to a block-diagonal form of the matrix $\mathbf{M}$. If the symmetry group of the system is finite, we obtain [see App. B for the details of symmetry reductions]

$$\det \mathbf{S}^{(N)}(k) = \left(\prod_{j=1}^{N} \det \mathbf{S}^{(1)}(j;k) \right) \frac{\prod_c (\mathrm{Det}\,(\tilde{\mathbf{M}}_{D_c}(k^*))^\dagger)^{d_c}}{\prod_c (\mathrm{Det}\,\tilde{\mathbf{M}}_{D_c}(k))^{d_c}} \,, \tag{23}$$

where the index c runs over all conjugacy classes and D_c denotes the c^{th} irreducible representation of dimension d_c of the symmetry group. The last formula represents the final result of our formal treatment of scattering systems consisting of N spherical scatterers. The scattering resonances corresponding to the c-th irreducible representation of the symmetry group are given by the zeros of $\mathrm{Det}\,\tilde{\mathbf{M}}_{D_c}(k)$ and they are d_c-fold degenerate.

In Sec. 4 it will be shown that all the formal manipulations that lead to Eqs. (22) and (23), and especially all the determinants appearing in it, are well defined if the number N of scatterers is finite and the scatterers do not overlap nor touch.

3.2 Connection to the Semiclassical Gutwiller-Voros Zeta-Function

The determinant of the characteristic matrix $\mathbf{M}$ is understood in terms of the cumulant expansion [3, 18], which can be formally obtained from Eqs. (15) and (16),

$$\begin{aligned} \mathrm{Det}\,\mathbf{M} &= \exp\{\mathrm{Tr}\,\log \mathbf{M}\} \equiv \exp\{\mathrm{Tr}\,\log(\mathbf{1}+\mathbf{W})\} \\ &= 1 + \mathrm{Tr}\,\mathbf{W} - \frac{1}{2}\left[\mathrm{Tr}\,(\mathbf{W})^2 - (\mathrm{Tr}\,\mathbf{W})^2\right] + \dots \,. \end{aligned} \tag{24}$$

The first line of the upper equation is only of formal character — especially it is not defined at the zeros of $\mathrm{Det}\,\mathbf{M}$. Nevertheless, it offers an easy way to remember the second line, which defines the determinant of $\mathbf{M}$, if $\mathbf{W}$ is trace class (see Ref. [3] and references therein).

In a semiclassical description the scattering resonances can be extracted from the zeros of the Gutzwiller-Voros zeta function, which formally can be written as [7, 8]

$$
\begin{aligned}
Z_{GV}(k;z) &= \exp\left\{ -\sum_p \sum_{r=1}^{\infty} \frac{1}{r} \frac{(z^{n_p} t_p)^r}{|\det(\mathbf{J}_p{}^r - \mathbf{1})|^{\frac{1}{2}}} \right\} \\
t_p &= \exp\left\{ i \left(\frac{S_p(k)}{\hbar} - \nu_p \frac{\pi}{2} \right) \right\} .
\end{aligned}
\tag{25}
$$

Here $\mathbf{J}_p$ denotes the monodromy matrix of the p-th primitive periodic orbit of topological length n_p, $S_p(k)$ and ν_p are the corresponding classical action and Maslov index, respectively. The sum over r takes into account the repeated traversals of the primitive periodic orbits. In the above expression, z is a book-keeping variable and the Gutzwiller-Voros zeta function has to be evaluated at $z = 1$. This expression is only of formal character, it has to be regulated. Expanding (25) in powers of z the curvature expansion is obtained,

$$
Z_{GV}(k;z) = 1 - z \sum_p \delta_{n_p,1} \frac{t_p}{\Gamma_{p,r=1}} - \frac{z^2}{2} c_2 + \ldots \tag{26}
$$

$$
\begin{aligned}
c_2 &= 2 \sum_p \sum_r \delta_{n_p r,2} \frac{1}{r} \frac{(t_p)^r}{\Gamma_{p,r}} - \sum_{p,p'} \delta_{n_p,1}\, \delta_{n_{p'},1} \frac{t_p t_{p'}}{\Gamma_{p,r=1} \Gamma_{p',r=1}} \\
\Gamma_{p,r} &\equiv |\det(\mathbf{J}_p{}^r - \mathbf{1})|^{\frac{1}{2}} = |\Lambda_{1,p} \Lambda_{2,p}|^{\frac{1}{2}} (1 - \Lambda_{1,p}{}^{-r})(1 - \Lambda_{2,p}{}^{-r}) .
\end{aligned}
\tag{27}
$$

The n-th curvature c_n contains all periodic orbits up to the topological length n. As can be seen from Eq. (27), the contribution of orbits of topological length n (> 1) gets reduced by pseudo-orbits, composed of shorter periodic orbits, of the same total length. Equations (25) and (26) (except for the last equality in the last line) are valid for two-dimensional N-disk systems as well as for three-dimensional N-sphere systems. In contrast to the well known two-dimensional case, in three dimensions the monodromy matrix, as being a 4×4-matrix, has two leading eigenvalues $|\Lambda_1|, |\Lambda_2| > 1$ [7]. For a generic periodic orbit in an N-sphere system the two leading eigenvalues are different. The most important exception is the only periodic orbit of the two-sphere-system, here Λ_1 and Λ_2 coincide. In N-sphere systems which have a two-dimensional analogue – this means that the centers of the N spheres are located all in one plane – one of the leading eigenvalues is given by the leading eigenvalue in the corresponding N-disk system while the other takes into account the instability of the periodic orbit against perturbations perpendicular to the plane. The lengths and Maslov indices of the periodic orbits in these N-sphere systems coincide with the corresponding quantities in the analogous N-disk system. As in the two-dimensional N-disk systems, orbits which are situated on the boundary of the fundamental domain require a special treatment [36, 37].

It is easy to see that the series of Eq. (24) has the same structure as the curvature expansion of the semiclassical Gutzwiller-Voros zeta function (26). Furthermore, the quantum-mechanical description of N-sphere scattering systems is analogous to the quantum-mechanical description of two-dimensional N-disk systems. In the treatment of N-disk systems a direct link between the quantum-mechanical and semiclassical descriptions has been established [3]. On the quantum-mechanical side this link is based on (24). Therefore we conjecture a similar direct link between quantum mechanics and semiclassics in N-sphere systems: The semiclassical limit of the cumulant expansion in the Plemej-Smithies form (see Ref.[35]) of $\mathrm{Det}\,\mathbf{M}$ is given by the curvature regulated Gutzwiller-Voros zeta function plus diffractional corrections,

$$\begin{aligned} \mathrm{Det}\,\mathbf{M}(k) &\quad \xrightarrow{\text{s.c.}} \quad \widetilde{Z}_{GV}(k)|_{\text{curv. reg.}} \\ \mathrm{Tr}\left(\mathbf{W}^n(k)\right) &\quad \xrightarrow{\text{s.c.}} \quad (-1)^n \sum_p \delta_{n_p r,n}\, n_p \frac{t_p(k)^r}{\Gamma_{p,r}} + \text{diffractional corrections.} \end{aligned} \tag{28}$$

Hence, the semiclassical limit of the n-th cumulant is given by the n-th curvature order in the Gutzwiller-Voros zeta function plus diffractional corrections. This direct link, which connects the quantum-mechanical and semiclassical descriptions, is valid for all complex k and not only for the isolated scattering resonance poles. We call it a direct link because it is not based on concepts characteristic to bound-state problems. So it is not based on any asymptotic limit of spectral densities (see Refs. [17] and [38]):

$$\lim_{b\to\infty} \left(N^{(N)}(k;b) - N^{(0)}(k;b) \right) = \frac{1}{2\pi} \mathrm{Im}\mathrm{Tr}\, \ln \mathbf{S}(k) \ , \tag{29}$$

where $N^{(N)}(k;b)$ and $N^{(0)}(k;b)$ are the integrated spectral densities belonging to two spherical bound systems, both of the same radius b, where one encircles the scattering region whereas the other doesn't (see Ref. [3] for a detailed discussion in the analogous two-dimensional N-disk systems). In fact, this formula is only correct in the double limit $\lim_{\epsilon\to 0}\lim_{b\to\infty}$ where a small positive imaginary part $i\epsilon$ has to be added to the wave number, before the limit $b \to \infty$ can be taken.

In Ref. [39] a structure similar to that of Eq. (24) of the characteristic determinant for generic two-dimensional systems was derived in a semiclassical description under the Fredholm theory.

4 Justification of the Previous Calculations

The derivation of the expression for the $\mathbf{S}$-matrix (14) and the derivation of its determinant in Sec. 3 are of a purely formal character since all the matrices involved are of infinite size. In this Section, we show that the calculations of the previous Section are mathematically sound. This discussion is of considerable conceptual importance. However, those readers who are mainly interested in the numerical results of our study are adviced to skip the present Section.

In the proofs that all the performed operations are well defined the so-called trace-class and Hilbert-Schmidt operators [35] play a central role. Trace class operators are those, in general, non-hermitian operators of a separable Hilbert-Space which have an absolutely

convergent trace in every orthonormal basis. An operator $\mathbf{B}$ belongs to the Hilbert-Schmidt class if $\mathbf{B}^\dagger\mathbf{B}$ is trace-class. Here we will not present all the proofs in detail. We refer to [3] where the corresponding problem in the two-dimensional N-disk scattering systems is treated. In that reference the most important properties of trace-class and Hilbert-Schmidt operators are listed: (i) any trace-class operator can be represented as the product of two Hilbert-Schmidt operators and any such product is trace-class; (ii) an operator $\mathbf{B}$ is already Hilbert-Schmidt, if the trace of $\mathbf{B}^\dagger\mathbf{B}$ is absolutely convergent in just one orthonormal basis; (iii) the linear combination of a finite number of trace-class operators is again trace-class; (iv) the adjoint of a trace-class operator is again trace-class; (v) the product of two Hilbert-Schmidt operators or of a trace-class and a bounded operator is trace-class and commutes under the trace; (vi) if $\mathbf{B}$ is trace-class, the determinant $\det(\mathbf{1}+z\mathbf{B})$ exists and is an entire function of z; (vii) the determinant is invariant under unitary transformations.

In close analogy to the results of Ref. [3] the following steps can be proven – provided that N is finite and that the spheres do not touch nor overlap:

(a) $\mathbf{D}^j$ is a trace-class matrix for all complex k. Also $\mathbf{C}^j$ is a trace-class matrix except at the isolated zeros of $h_l^{(1)}(ka_j)$, where l is a nonnegative integer and $j=1,\ldots,N$. (One very simple way to prove this is to transform $\mathbf{D}^j$ and $\mathbf{C}^j$ into the eigenbasis of the $j^{\,\rm th}$ sphere, see Eq.(20). In that eigenbasis both matrices become diagonal and the trace-class property can easily be checked by summing up the moduli of their eigenvalues. In the same way it can be checked that the one-sphere $\mathbf{T}$-matrix $\mathbf{S}^{(1)}(j;k)-\mathbf{1}$ is trace-class, too.)

(b) Therefore the product $\mathbf{D}^j\mathbf{C}^{j'}$ is of trace-class as long as N is finite and $\mathbf{C}^{j'}$ is trace-class.

(c) $\mathbf{M}^{jj'}-\delta^{jj'}\mathbf{1}=\mathbf{W}^{jj'}$ is trace-class, except at the same k-values mentioned in **(a)**. This can be proved by rewriting $\mathbf{W}^{jj'}$ as the product of two matrices, $\mathbf{G}^{jj'}$ and a diagonal matrix $\mathbf{H}^{jj'}$, which both can be shown — as in Ref.[3] — to be Hilbert-Schmidt matrices:

$$
\begin{aligned}
\mathbf{G}^{jj'}_{lm,l'm'} &= (1-\delta^{jj'})\left(\frac{a_j}{a_{j'}}\right)^2\sqrt{4\pi}\frac{(-1)^m}{(2l'+1)^{\frac{3}{2}}}\,\frac{j_l(ka_j)}{\sqrt{h^{(1)}_{2l'}(k\alpha a_{j'})}} \\
&\quad\times\sum_{l_1=0}^{\infty}\sum_{\tilde m=-l'}^{l'} i^{l_1+l'-l}\sqrt{(2l+1)(2l_1+1)(2l'+1)} \\
&\quad\times\begin{pmatrix} l_1 & l' & l\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l_1 & l' & l\\ m-\tilde m & \tilde m & -m\end{pmatrix} \\
&\quad\times h^{(1)}_{l_1}(kR_{jj'})Y_{l_1,m-\tilde m}(\hat R^{(j)}_{jj'})D^{l'}_{m'\tilde m}(j,j')
\end{aligned}
\tag{30}
$$

and

$$
\mathbf{H}^{j'j''}_{l'm',l''m''}=\delta^{j'j''}\delta_{l'l''}\delta_{m'm''}\,(2l'+1)^{\frac{3}{2}}\frac{\sqrt{h^{(1)}_{2l'}(k\alpha a_{j'})}}{h^{(1)}_{l'}(ka_{j'})}\;, \tag{31}
$$

where $\alpha > 2$. This inequality is the reason that our proofs exclude the case of touching spheres. In fact, the geometry of the N scatters must be such that the inequality $\frac{\alpha}{2}a_j + a_{j'} < R_{jj'}$ is valid for all pairs j and j'.

(d) Therefore $\mathbf{M}$ is bounded.

(e) $\mathbf{M}$ is invertible everywhere where $\mathrm{Det}\,\mathbf{M}$ is defined and nonzero (which excludes a countable number of isolated points in the lower k-plane). Especially, $\mathbf{M}$ is invertible on the real k axis. Therefore, the matrix $\mathbf{M}^{-1}$ is bounded on the real k axis as well.

(f) $\mathbf{C}^j(\mathbf{M}^{-1})^{jj'}\mathbf{D}^{j'}$, $\mathbf{M}^{-1}\mathbf{DC}$, are all of trace-class (except at the isolated points mentioned in **(a)** and **(e)** as they are the product of a (finite number of) bounded and trace-class matrices, and $\mathrm{tr}\,[(\mathbf{C}^j(\mathbf{M}^{-1})^{jj'}\mathbf{D}^{j'})^n] = \mathrm{Tr}\,[(\mathbf{M}^{-1}\mathbf{DC})^n]$ exists (note the matrices on the l.h.s. are labeled by the index pairs l, m, whereas the ones on the r.h.s. are labeled by the index triples j, l, m).

(g) $\mathbf{M} - i\mathbf{DC} - \mathbf{1}$ is of trace-class because of **(b)** and **(c)** and the rule that the sum of two trace-class matrices is again trace-class.

The properties **(a)** – **(g)** ensure that the derivation of Eq. (17) starting from (14) is correct. Because of **(e)** formula (14) makes sense (also on the real k-axis). Under the assumption that the matrix $\mathbf{A}$, which characterizes the gradient of the wave function on the surfaces of the scatterers (see Eq. (8)), is bounded, the determinant of $\mathbf{S}$ on the basis of (12) is defined. Now it is easy to see (using property **(a)** and **(c)**) that all determinants appearing in the formula (22) exists and that the unitary transformations leading to (23) are justified.

5 Numerical Results

We have calculated the scattering resonances of the three simplest and most symmetrical N-sphere systems. These systems consist of two, three and four hard spheres, respectively, which all have the *same* radius $a_j \equiv a$ and the *same* center-to-center separation $R_{ij} \equiv R$: two non-touching spheres (two spheres), three spheres at the corners of an equilateral triangle (three spheres) and four spheres at the corners of a regular tetrahedron (four spheres). In all cases we have chosen the ratio R/a to have the fixed value 6 in order to be able to compare with older two and three-disk calculations.

The quantum-mechanical resonances have been calculated as the zeros of the determinant of the characteristic matrix $\mathbf{M}$ in a finite basis corresponding to angular momenta from $l = 0$ up to a certain maximum value which depends on the wave number k. We checked the accuracy of the results against a further enhancement of the basis. This method is applicable, as the trace class property of $\mathbf{M} - \mathbf{1}$ guarantees the existence of the limit. The zeros in the complex k-plane were determined with the help of a Newton-Raphson routine.

The semiclassical resonances have been calculated as the zeros of the curvature regulated Gutzwiller-Voros zeta function without diffractional corrections. In the two-sphere and three-sphere systems the zeta function can be easily constructed under the techniques described in Sec. 3, with the input from the corresponding two-disk and three-disk systems, respectively.

The four-sphere-system is the simplest N-sphere scattering system which does not have a two-dimensional analogue. In this case, only the three fundamental periodic orbits of topological length 1 have been determined so far.

In Sec. 5.1, we discuss the quantum mechanically calculated resonances of the N-sphere systems. They are compared to those of the two-dimensional N-disk systems in Sec. 5.2. In Sec. 5.3, we compare the quantum mechanical and the semiclassical results for the N-sphere systems.

5.1 Quantum Mechanically Calculated Resonances

In Secs. 5.1.1, 5.1.2 and 5.1.3 we discuss the two-, three and four-sphere systems, respectively.

5.1.1 Two Spheres

The scatterer configuration is shown in Fig. 1. This system has a continuous symmetry, the rotational symmetry about the axis which joins the centers of the spheres. Hence, the corresponding symmetry group, $D_{\infty h}$, is infinite and has 4 one-dimensional irreducible representations and an infinite number of two-dimensional ones [40]. From the 4 one-dimensional representations only two are present due to the lack of any inner structure of the two spherical scatterers.

The blocks of the symmetry reduced **M**-matrix are given by:

one-dimensional representations (with $m = 0$):

$$\begin{aligned}
\tilde{\mathbf{M}}_{ll'}(D) &= \delta_{ll'} + (-1)^c (-1)^{l'} i^{l'-l} \frac{j_l(ka)}{h^{(1)}_{l'}(ka)} \sqrt{(2l+1)(2l'+1)} \\
&\quad \times \sum_{l_1=0}^{\infty} i^{l_1} (2l_1+1) \left(\begin{pmatrix} l_1 & l' & l \\ 0 & 0 & 0 \end{pmatrix} \right)^2 h^{(1)}_{l_1}(kR) \\
c &= \begin{cases} 0 & \text{for } D_c = A_{1g} \\ 1 & \text{for } D_c = A_{1u} \end{cases}
\end{aligned}$$

two-dimensional representations:

$$\begin{aligned}
\tilde{\mathbf{M}}_{ll'}(D) &= \delta_{ll'} + (-1)^c (-1)^{l'} i^{l'-l} \frac{j_l(ka)}{h^{(1)}_{l'}(ka)} \sqrt{(2l+1)(2l'+1)} \\
&\quad \times \sum_{l_1=0}^{\infty} i^{l_1} (2l_1+1) \begin{pmatrix} l_1 & l' & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l' & l \\ 0 & m & -m \end{pmatrix} h^{(1)}_{l_1}(kR) \\
c &= \begin{cases} 0 & \text{for } D_c = E_{mg} \\ 1 & \text{for } D_c = E_{mu} \end{cases} \\
l, l' &\geq m > 0 \,,\ m \text{ fixed.}
\end{aligned}$$

The degeneracy-degree of the resonances coincides with the dimensionality of the representation. As a consequence of the continuous rotational symmetry, $|m|$ is a good quantum number and there are two irreducible representations corresponding to each value of $|m|$.

The numerically calculated resonances of the two-sphere-system are shown in Figs. 4-6. The leading resonances of Fig. 4 form a regular structure which we call a Gutzwiller-band. The suppressed resonances do not build up such a regular structure; we say they lie in a diffraction-band. This terminology is chosen in analogy to the similar results found in two-dimensional problems (scattering from N hard disks) [2, 3, 18, 23, 24]. The resonances corresponding to increasing $|m|$ become increasingly suppressed. This is due to the centrifugal barrier, which in cylindrical coordinates reads m^2/r^2.

In Fig. 5 we see that the leading resonances of the $|m| = 1$ representations for small real parts of k lie in the diffraction band. For real parts of k bigger than approximately $10/a$ two Gutzwiller bands build up, which are shifted by half a spacing in Re k but coincide in their values of Im k.

5.1.2 Three Spheres

The scatterer configuration of the three-sphere-system is shown in fig 2. The symmetry group D_{3h} consists of 12 elements. It has four one-dimensional and two two-dimensional representations [40].

The symmetry reduced expressions for the distinct blocks of the **M**-matrix are given as follows.

There are four one-dimensional representations ($0 \leq m,\, m'$):

$$\tilde{\mathbf{M}}_{lm,l'm'}(A_1{}') = \begin{cases} 0 & ,\ (l+m) \text{ or } (l'+m') \text{ odd} \\ \mathbf{E}_{lm,l'm'}(\alpha = 0) & ,\ \text{otherwise} \end{cases} \tag{32}$$

$$\tilde{\mathbf{M}}_{lm,l'm'}(A_1{}'') = \begin{cases} 0 & ,\ (l+m) \text{ or } (l'+m') \text{ even} \\ \mathbf{E}_{lm,l'm'}(\alpha = 1) & ,\ \text{otherwise} \end{cases} \tag{33}$$

$$\tilde{\mathbf{M}}_{lm,l'm'}(A_2{}') = \begin{cases} 0 & ,\ (l+m) \text{ or } (l'+m') \text{ odd} \\ \mathbf{E}_{lm,l'm'}(\alpha = 1) & ,\ \text{otherwise} \end{cases} \tag{34}$$

$$\tilde{\mathbf{M}}_{lm,l'm'}(A_2{}'') = \begin{cases} 0 & ,\ (l+m) \text{ or } (l'+m') \text{ even} \\ \mathbf{E}_{lm,l'm'}(\alpha = 0) & ,\ \text{otherwise} \end{cases} \tag{35}$$

$$
\begin{aligned}
\mathbf{E}_{lm,l'm'}(\alpha) &= \delta_{ll'}\delta_{mm'} \\
&\quad + 2g_m g_{m'}\sqrt{4\pi}(-1)^m i^{l'-l}\frac{j_l(ka)}{h^{(1)}_{l'}(ka)} \\
&\quad \times \sum_{l_1=0}^{\infty} i^{l_1} h^{(1)}_{l_1}(kR)\sqrt{(2l+1)(2l'+1)(2l_1+1)}\begin{pmatrix} l_1 & l' & l \\ 0 & 0 & 0 \end{pmatrix} \\
&\quad \times \left\{ \begin{pmatrix} l_1 & l' & l \\ m-m' & m' & -m \end{pmatrix} \cos\left(\frac{\pi}{6}(5m-m')\right) Y_{l,m-m'}(\frac{\pi}{2},0) \right. \\
&\quad \left. + (-1)^{\alpha+m'} \begin{pmatrix} l_1 & l' & l \\ m+m' & -m' & -m \end{pmatrix} \cos\left(\frac{\pi}{6}(5m+m')\right) Y_{l,m+m'}(\frac{\pi}{2},0) \right\} \\
g_m &= \begin{cases} 1 & , \; m>0 \\ \frac{1}{\sqrt{2}} & , \; m=0. \end{cases}
\end{aligned}
$$

In addition, there are two two-dimensional representations (m, m' integer):

$$
\tilde{\mathbf{M}}_{lm,l'm'}(E') = \begin{cases} 0 & , \; (l+m) \text{ or } (l'+m') \text{ odd} \\ \mathbf{F}_{lm,l'm'} & , \; \text{otherwise} \end{cases} \tag{36}
$$

$$
\tilde{\mathbf{M}}_{lm,l'm'}(E'') = \begin{cases} 0 & , \; (l+m) \text{ or } (l'+m') \text{ even} \\ \mathbf{F}_{lm,l'm'} & , \; \text{otherwise} \end{cases} \tag{37}
$$

with

$$
\begin{aligned}
\mathbf{F}_{lm,l'm'} &= \delta_{ll'}\delta_{mm'} \\
&\quad + 2\sqrt{4\pi} i^{l'-l}(-1)^m \frac{j_l(ka)}{h^{(1)}_{l'}(ka)} \\
&\quad \times \sum_{l_1=0}^{\infty} i^{l_1}\sqrt{(2l+1)(2l'+1)(2l_1+1)}\begin{pmatrix} l_1 & l' & l \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1 & l' & l \\ m-m' & m' & -m \end{pmatrix} \\
&\quad \times h^{(1)}_{l_1}(kR) Y_{l_1,m-m'}(\frac{\pi}{2},0)\cos\left(\frac{\pi}{6}(5m-m'-4)\right) \; .
\end{aligned}
$$

The numerically calculated resonances of the ${A_1}'$ and ${A_1}''$ symmetry classes are shown in Fig. 7. The ${A_1}''$ resonances are suppressed compared with the ${A_1}'$ resonances, because the wave function has to vanish in the plane of the triangle due to the symmetry (see character table of D_{3h} in Ref. [40]). This is the plane which contains all geometric periodic orbits of the three-sphere-system, which play the dominant role in a semiclassical treatment in the considered wave number regime. The resonances of the ${A_2}'$, ${A_2}''$ and E', E'' symmetry classes show a similar behaviour.

5.1.3 Four Spheres

The scatterer configuration of the four-sphere-system is shown in fig 3. Compared with the two- and three-sphere-systems this is the first genuine three-dimensional scattering system since the scatterers (and therefore the set of all geometric periodic orbits) do not lie in a plane.

The symmetry group T_d has 24 elements. It has 2 one-dimensional, 1 two-dimensional and 2 three-dimensional irreducible representations [40]. Here only the one-dimensional representations are considered. The corresponding blocks of the symmetry reduced **M**-matrix are given by:

$$\begin{aligned}
\tilde{\mathbf{M}}_{lm,l'm'}(D) &= \delta_{ll'}\delta_{mm'} \\
&\quad + \frac{3}{2}\sqrt{4\pi}\, i^{l'-l}\frac{j_l(ka)}{h^{(1)}_{l'}(ka)} g_m g_{m'} \\
&\quad \times \sum_{\tilde{l}=0}^{\infty}\sum_{M=-l'}^{l'} i^{\tilde{l}} h^{(1)}_{\tilde{l}}(kR)\sqrt{(2l+1)(2l'+1)(2\tilde{l}+1)}\begin{pmatrix}\tilde{l} & l' & l\\ 0 & 0 & 0\end{pmatrix} \\
&\quad \times (-1)^M\left(d^{l'}_{m'M}(\beta_0) + (-1)^{Q+m'} d^{l'}_{-m',M}(\beta_0)\right) \\
&\quad \times \Bigg[(-1)^m Y_{\tilde{l},m-M}(\theta_0,0)\begin{pmatrix}\tilde{l} & l' & l\\ m-M & M & -m\end{pmatrix} \\
&\qquad + (-1)^Q Y_{\tilde{l},-m-M}(\theta_0,0)\begin{pmatrix}\tilde{l} & l' & l\\ -m-M & M & m\end{pmatrix}\Bigg] \qquad (38)\\
Q &= \begin{cases} 0 & \text{for } D = A_1\\ 1 & \text{for } D = A_2\end{cases} \\
g_m &= \begin{cases} \sqrt{2} & \text{for } m = 0\\ 1 & \text{for } m = 3,6,9,\ldots,l\\ 0 & \text{otherwise}\end{cases} \\
d^j_{mm'}(\beta) &\equiv \langle jm\,|e^{-i\beta J_y}|jm'\rangle \\
\cos(\theta_0) &= -\frac{2}{\sqrt{6}} \quad , \quad \sin(\theta_0) = \frac{1}{\sqrt{3}} \\
\cos(\beta_0) &= -\frac{1}{3} \quad , \quad \sin(\beta_0) = \frac{2}{3}\sqrt{2}
\end{aligned}$$

The numerically calculated A_1-resonances are shown in Fig. 8.

A comparison of the first leading Gutzwiller resonances of the two-, three- and four-sphere-systems shows that the spacing in the real part of k in the resonance band slightly decreases if one looks first at the two-sphere, then at the three-sphere and finally at the four-sphere system. This spacing is governed by the inverse length of the (averaged) periodic orbits of topological length one in the fundamental domain. In the two-sphere case there exists only one periodic orbit. The three-sphere system has in addition to this orbit one

further fundamental periodic orbit, which in the global domain corresponds to an equilateral triangle spanned inbetween the three scatterers. The length in the fundamental domain of this second periodic orbit is only slightly bigger than that of the two-sphere orbit. In the four-sphere system there are three fundamental periodic orbits: The two orbits of the three-sphere system and an additional orbit which touches all four spheres in the global domain and which again it slightly bigger than the other two when measured in the fundamental domain. Thus the average length of the fundamental orbits increases with the increasing number of spheres.

As far as the imaginary parts of the first leading Gutzwiller resonances of the two-, three- and four-sphere-systems are concerned, we see that the two-sphere resonances are slightly more suppressed than the three-sphere resonances, which are in turn slightly suppressed as compared to the four-sphere-resonances. This is due to the fact that the addition of one further sphere increases the probability that the particle is rescattered to the other spheres and therefore trapped for a longer time in the scattering region.

5.2 Comparison of the Quantum Mechanically Calculated Resonances of N-Sphere and N-Disk Systems

If the centers of the spheres of a given N-sphere configuration lie all in one plane, there exists an analogous two-dimensional N-disk scattering system. In this case it makes sense to compare directly these analogue systems, although they differ in their dimensionality: they have in common the entire set of classically allowed periodic orbits which play the dominant role in a semiclassical description in the wave number regime considered here [14, 18, 26].

In Fig. 9 the resonances of the totally symmetric representations of the two-sphere and two-disk systems are shown. In both cases the leading resonances lie in Gutzwiller bands. Suppressed resonances form diffraction bands. However, in the two-disk system a sub-leading Gutzwiller band seems to appear for larger wave numbers ($\mathrm{Re}\, k > 15/a$). The leading resonances in the two-sphere and two-disk systems have the same real part, but the whole two-sphere band is shifted down into the negative complex k plane, because the only existing geometrical periodic orbit is more instable in the three-dimensional case than in the two-dimensional one. In the semiclassical formulae the higher instability is easily explained by the existence of a second leading eigenvalue of the monodromy matrix (see Sec. 3.2). There is no such coincidence in the real parts of the resonances of the diffraction bands. This behaviour is also expected from a semiclassical point of view as the diffractional orbits in both cases act on different manifolds.

In Fig. 10 the resonances of the totally symmetric representations of the three-sphere and three-disk systems are shown. In both cases the leading resonances lie in Gutzwiller bands. Suppressed resonances form diffraction bands. As in the two-scatterer systems, we find a good agreement between the real parts of the sphere and disk resonances (which is getting better for larger wave numbers) while the whole three-sphere Gutzwiller band is shifted to smaller imaginary parts by the same amount as in the two-scatterer case. The same behaviour is observed for the two-dimensional representations E' (three-sphere) and E (three-disk), respectively.

In summary we see, without using the results of any semiclassical calculation, that the

leading resonances in the analogous two- and three-dimensional N-scatterer systems are dominated by the contribution of the geometric periodic orbits. In contrast, the suppressed resonances show no one-to-one correspondence between the disk and sphere resonances. So the conclusion, which so far is only based on the presented quantum-mechanical data, is that the suppressed resonances are due to diffractional effects, which should be different in two and three dimensions.

5.3 Comparison of Quantum Mechanically and Semiclassically Calculated Resonances in N-Sphere Systems

As described in Sec. 3.2, it is possible to transfer the well developed techniques of calculating scattering resonances under the periodic orbit approximation with only classically allowed orbits [14, 17, 18] from N-disk systems to scattering problems with N hard spheres in three dimensions.

In particular, the semiclassical resonances of the two-sphere-system are given by the zeros of the following spectral zeta function,

$$Z(k) = \prod_{c=0}^{\infty} Z_{c=|m|}^{g/u}(k) = \prod_{m=-\infty}^{\infty} \prod_{n=0}^{\infty} \left(1 \pm \frac{e^{ik(R-2a)}}{|\Lambda_0|\Lambda_0^{|m|+2n}} \right) , \tag{39}$$

where the $\pm$ sign refers to the g/u representations and $Z_{|m|}$ contains all terms of a given $|m|$ in the last expression. Λ_0 is the leading eigenvalue of the monodromy matrices of the 2-disk and the two-sphere systems. In the three-dimensional case this eigenvalue is two-fold degenerate.

Also in the three-sphere system the semiclassical zeta function can be constructed from the corresponding expression for the two-dimensional three-disk system. As all periodic orbits lie in one plane, the 4×4 monodromy matrix decomposes into blocks of 2×2 matrices, where the off-diagonal blocks vanish. One block describes the motion in the plane and it is given by the monodromy matrix of the three-disk system. The other block describes the motion perpendicular to the plane and can be constructed from the same section lengths l_i, local curvature radii ρ_i and scattering angles θ_i as in the three-disk system. The only difference is that the matrix elements of the 2×2 dimensional reflecting matrix of Ref.[17] change to [41]

$$\begin{pmatrix} -1 & -2/[\rho_i \cos(\theta_i)] \\ 0 & -1 \end{pmatrix} \longrightarrow \begin{pmatrix} 1 & 2\cos(\theta_i)/\rho_i \\ 0 & 1 \end{pmatrix} , \tag{40}$$

whereas the translational matrices stay as

$$\begin{pmatrix} 1 & 0 \\ l_i & 1 \end{pmatrix} .$$

Note that in the 2-scatterer cases the angles θ_i are always zero.

In Fig. 11 the quantum-mechanically and semiclassically calculated resonances of the completely symmetric representation of the two-sphere system are shown. The agreement between the quantum-mechanical and semiclassical data in the leading Gutzwiller band is very good

except for the first few resonances located at small real parts of the wave number k. In contrast, the suppressed quantum resonances situated in the diffraction band cannot be described by these semiclassical calculations. Note that the agreement of the leading resonances calculated quantum-mechanically and semiclassically is already very good at quite small real parts of k. For increasing $\mathrm{Re}\, k$ this agreement improves.

Also the quantum-mechanical and semiclassical resonances of the completely symmetric representation of the three-sphere-system have been calculated. Again, we find a good agreement between the quantum-mechanical and semiclassical data in the case of the leading Gutzwiller band except for the first few low-lying resonances. As in the two-sphere case the suppressed quantum resonances of the diffraction band cannot be described by these semiclassical calculations.

In the four-sphere-system, we have only determined the three fundamental periodic orbits so far. Even in this case a comparison between the zeros of the quantum determinant $\mathrm{Det}\, \mathbf{M}$ calculated via the cumulant expansion (24) which has been truncated after the first cumulant shows an agreement between the quantum and semiclassical leading resonances.

6 Conclusions

We presented a quantum mechanical and a semiclassical discussion of a chaotic system in three dimensions. As a model, we chose the scattering of a point particle on N hard spheres in three dimensions. We showed that certain methods which were developed in the framework of two-dimensional systems can be extended to three dimensions in a straightforward way. Within the framework of stationary scattering theory and using Green's theorem an expression for the determinant of the scattering matrix $\mathbf{S}$ was derived. In order to determine the scattering resonances it suffices to look for the poles of the determinant of the $\mathbf{S}$-matrix. The determinant of the $\mathbf{S}$-matrix of the entire N-sphere scattering system splits up into a coherent and an incoherent part. The coherent part is given by the ratio of the determinants of the hermitian conjugate and of the characteristic matrix $\mathbf{M}$ itself, where $\mathbf{M}$ contains the information on the geometry of the entire N-scatterer configuration. The incoherent part consists of the product of the N determinants of the 1-scatterer $\mathbf{S}$-matrices, each expressed in a coordinate system whose origin lies in the center of the individual scatterer. The expression for $\det \mathbf{S}^{(N)}$ respects the unitarity of the scattering matrix and guarantees a unitary semiclassical limit without any resummation techniques a la Berry and Keating [6]. The scattering resonances are given by the zeros of the determinant of $\mathbf{M}$. The poles of the incoherent part of $\det \mathbf{S}^{(N)}$ get canceled by the poles of $\mathrm{Det}\, \mathbf{M}$. A proof was given that all the formal manipulations in our derivations are allowed and that the final expression for $\det \mathbf{S}^{(N)}$ is well defined provided that the number of scatterers is finite and that they do not touch nor overlap. Similar results have been found in the description of two-dimensional N-disk scattering systems [2, 3].

We conjecture the following direct link between the quantum-mechanical and semiclassical descriptions of N-sphere scattering systems: The semiclassical limit of $\mathrm{Tr}\,(\mathbf{W}^n)$, $\mathbf{W} \equiv \mathbf{M} - \mathbf{1}$, is given by those terms of the curvature regulated Gutzwiller-Voros zeta function which correspond to periodic orbits of total topological length $n = n_p r$ (r denotes the number of

repeats), each weighted with the topological length n_p of the underlying primitive periodic orbit, plus diffractional corrections. As the determinant of $\mathbf{M}$ is given by the cumulant expansion, this means that the semiclassical limit of the n-th cumulant of $\mathrm{Det}\,\mathbf{M}$ is given by the n-th curvature order of the Gutzwiller-Voros zeta function plus diffractional corrections. This connection holds for all complex wave numbers. It is direct, as it does not rely on the subtraction of the (integrated) spectral densities of two equally sized infinitely large *bounded* reference systems – one containing the N-sphere scatterer and the other not [17, 38]. Again this is analogous to the results found in N-disk scattering systems [3].

Qualitatively, the distribution of the quantum-mechanically calculated resonances of N-sphere systems is similar to the known results of N-disk systems [2, 3]. Comparing the computed resonances of analogous N-sphere and N-disk systems, which have all the geometric periodic orbits in common, we see that the leading Gutzwiller resonances have the same real part but the whole resonance band of the three-dimensional system is shifted to smaller imaginary parts. This is due to the increased instability of the geometrical periodic orbits in the three-dimensional case. In the case of the suppressed resonances located in diffraction bands there is no such correspondence. The comparison of quantum-mechanically and semiclassically calculated N-sphere resonances shows qualitatively the same behaviour as in the two-dimensional N-disk systems.

The semiclassical investigation of N-sphere scattering systems is still a sparsely studied field. The description of diffractional corrections could be the subject of future projects. In this context an investigation of N-sphere systems in which the sphere separation is much bigger than the radii of the scatterers would be of interest, too, because diffraction effects should become more important. Also the opposite case with configurations of almost touching scatterers provides an interesting system in which bound states might develop. Another important point is a further investigation of the here conjectured link between the quantum-mechanical and semiclassical descriptions.

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A Details of the Calculation of the Scattering Matrix

We distinguish between the two possible cases defined in Sec. 2.2.

First case: $\vec{r}\,' \equiv \vec{r}_j \in$ boundary of the $j^{\text{ th}}$ scatterer
Green's theorem can be written in the form

$$0 = I_\infty^j + \sum_{j'=1}^{N} I_{j'}^j \;, \tag{41}$$

where the integrals are given by

$$\begin{aligned} I_\infty^j &= \int_{\partial_\infty V} d\vec{a} \cdot [\psi_{lm}^k(\vec{a}) \vec{\nabla} G(\vec{a}, \vec{r}_j) - G(\vec{a}, \vec{r}_j) \vec{\nabla} \psi_{lm}^k(\vec{a})] & (42) \\ I_{j'}^j &= -\int_{\partial_{j'} V} d\vec{a} \cdot G(\vec{a}, \vec{r}_j) \vec{\nabla} \psi_{lm}^k(\vec{a}) \;. & (43) \end{aligned}$$

The integrals defined in Eqs. (42) can be worked out in a straightforward calculation, we arrive at

$$\begin{aligned} I_\infty^j &= -\sqrt{4\pi}^5 \sum_{l_1, l_2=0}^{\infty} \sum_{\tilde{m}, m_2=-l_2}^{l_2} (-1)^m i^{l_1+l_2} \sqrt{(2l+1)(2l_1+1)(2l_2+1)} \\ &\quad \times j_{l_1}(ks_j) j_{l_2}(ka_j) \begin{pmatrix} l_1 & l_2 & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ m-m_2 & m_2 & -m \end{pmatrix} \\ &\quad \times Y_{l_1, m-m_2}(\hat{s}_j) Y_{l_2, \tilde{m}}(\hat{a}_j^{(j)}) D_{\tilde{m} m_2}^{l_2}(gl, j) \;, & (44) \\ I_j^j &= 4\pi i k \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{l'} a_j^2 A_{lm, l'm'}^j \, j_{l'}(ka_j) \, h_{l'}^{(1)}(ka_j) \, Y_{l'm'}(\hat{a}_j^{(j)}) \;, & (45) \\ I_{j'}^j &= \sqrt{4\pi}^3 i k a_{j'}^2 \sum_{l', l_1, l_2=0}^{\infty} \sum_{m'=-l'}^{l'} \sum_{m_2, \tilde{m}=-l_2}^{l_2} (-1)^{m'} i^{l_1+l_2-l'} \, \mathbf{A}_{lm, l'm'}^{j'} \\ &\quad \times \sqrt{(2l'+1)(2l_1+1)(2l_2+1)} \begin{pmatrix} l_1 & l_2 & l' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l' \\ m'-m_2 & m_2 & -m' \end{pmatrix} \\ &\quad \times j_{l'}(ka_{j'}) \, j_{l_2}(ka_j) \, h_{l_1}^{(1)}(kR_{j'j}) Y_{l_1, m'-m_2}(\hat{R}_{j'j}^{(j')}) \, Y_{l_2 \tilde{m}}(\hat{a}_j^{(j)}) \, D_{\tilde{m} m_2}^{l_2}(j', j) \;. & (46) \end{aligned}$$

In the derivation we made use of the addition theorems for Bessel functions,

$$\begin{aligned} i^l j_l(kr) Y_{lm}(\hat{r}) &= \sqrt{4\pi} \sum_{l_1, l_2=0}^{\infty} \sum_{m_1=-l_1}^{l_1} (-1)^m i^{l_1+l_2} \\ &\quad \times \sqrt{(2l+1)(2l_1+1)(2l_2+1)} j_{l_1}(ks) \, j_{l_2}(ka) \\ &\quad \times \begin{pmatrix} l_1 & l_2 & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m-m_1 & -m \end{pmatrix} Y_{l_1 m_1}(\hat{s}) Y_{l_2, m-m_1}(\hat{a}), & (47) \\ \vec{r} &= \vec{s} + \vec{a} \;, \end{aligned}$$

and Hankel functions [30],

$$
\begin{aligned}
i^l h_l^{(1)}(kr) Y_{lm}(\hat{r}) &= \sqrt{4\pi} \sum_{l_1,l_2=0}^{\infty} \sum_{m_1=-l_1}^{l_1} (-1)^m i^{l_1+l_2} \\
&\quad \times \sqrt{(2l+1)(2l_1+1)(2l_2+1)}\, h_{l_1}^{(1)}(ks) j_{l_2}(ka) \\
&\quad \times \begin{pmatrix} l_1 & l_2 & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m-m_1 & -m \end{pmatrix} Y_{l_1 m_1}(\hat{s}) Y_{l_2, m-m_1}(\hat{a}), \quad (48) \\
\vec{r} &= \vec{s} + \vec{a} \quad , \quad s > a \, ,
\end{aligned}
$$

which can be easily proven using $e^{i\vec{k}\cdot\vec{r}} = e^{i\vec{k}\cdot\vec{s}} e^{i\vec{k}\cdot\vec{a}}$ and the known properties of Bessel and Hankel functions [30]. We use the definition of Ref. [31] for the $3j$-symbols.

For large distances from the scatterer configuration we use the following asymptotic expressions for Hankel-functions [30] ($kr \to \infty$),

$$
h_l^{(2)}(kr) \sim \frac{1}{kr} e^{-i(kr - \frac{l+1}{2}\pi)} \, , \quad h_l^{(1)}(kr) \sim \frac{1}{kr} e^{+i(kr - \frac{l+1}{2}\pi)} \, . \tag{49}
$$

In changing coordinate systems we adopt the definitions of Rose [42] for the Euler angles and the irreducible representations of the rotational group, e.g.,

$$
D^j_{m'm}(\alpha\beta\gamma) = \langle jm' | e^{-i\alpha J_z} e^{-i\beta J_y} e^{-i\gamma J_z} | jm \rangle \, ,
$$

and $D^l_{m'm}(gl, j)$ denotes the corresponding quantity where the Euler angles describe the rotation of the axes of the (j)-system in those of the global system. For the spherical harmonics Y_{lm} we adopt the usual definition.

In particular, in the calculation of I^j_∞ the integration is performed in the global coordinate system. The Green's function are evaluated under the asymptotic expression (49) and finally the addition theorem (47) is applied and the coordinate system is changed. This leads to Eq. (44). In the calculation of I^j_j the integration is performed in the (j)-system. One easily obtains Eq. (45). In the calculation of $I^j_{j'}$, $j \neq j'$, we first perform the angular integration in the (j')-system. Then the addition theorem (48) is used and finally the coordinate system is changed. We get Eq. (46).

The expressions (44) to (46) are already written in a form $\sum_{lm} \cdots Y_{lm}(\hat{a}^{(j)}_j)$. It is now easy to see that Eq. (41), written as $-I^j_\infty = \sum_{j'=1}^N I^j_{j'}$, represents an equality between functions defined on the surfaces of the j-th scatterer and that it becomes

$$
\sum_{l_2,m_2} \tilde{\mathbf{C}}^j_{lm,l_2m_2} Y_{l_2m_2}(\hat{a}^{(j)}_j) = \sum_{l_2,m_2} \sum_{j',l',m'} \mathbf{A}^{j'}_{lm,l'm'} \tilde{\mathbf{M}}^{j'j}_{l'm',l_2m_2} Y_{l_2m_2}(\hat{a}^{(j)}_j) \, . \tag{50}
$$

We have obtained an equality between the coefficients appearing in the last equation up to a transformation of the form **C' ≡ CE = AME ≡ AM'**. Because of the reasons already discussed in Secs. 2 and 4 we write the characteristic matrix as $\mathbf{M} = \mathbf{1} + \mathbf{W}$ where the diagonal entries of $\mathbf{W}$ vanish. With these definitions we obtain Eqs. (9)–(11).

Second case: $\vec{r}\,' \in V$, r' large
According to (7) we obtain

$$\psi^k_{lm}(\vec{r}\,') = -\frac{1}{4\pi}\left(I^{\vec{r}\,'}_\infty + \sum_{j=1}^N I^{\vec{r}\,'}_j\right) \tag{51}$$

where the integrals are given by

$$\begin{aligned} I^{\vec{r}\,'}_\infty &= \int_{\partial_\infty V} d\vec{a}\cdot(\psi^k_{lm}(\vec{a})\vec{\nabla}G(\vec{a},\vec{r}\,') - G(\vec{a},\vec{r}\,')\vec{\nabla}\psi^k_{lm}(\vec{a})) && (52)\\ I^{\vec{r}\,'}_j &= -\int_{\partial_j V} d\vec{a}\cdot G(\vec{a},\vec{r}\,')\vec{\nabla}\psi^k_{lm}(\vec{a}) && (53)\end{aligned}$$

which yields Eq. (51) and thus determines the components of the wave function. The evaluation of the integrals yields

$$\begin{aligned} I^{\vec{r}\,'}_\infty &= -16\pi^2 i^l j_l(kr')Y_{lm}(\hat{r}') && (54)\\ I^{\vec{r}\,'}_j &= (4\pi)^{\frac{3}{2}} ika_j^2 \sum_{l'=0}^\infty \sum_{m'=-l'}^{l'} \sum_{l_1,l_2=0}^\infty \sum_{m_1=-l_1}^{l_1} (-1)^{m'+l_2} i^{l_1+l_2-l'} \\ &\times \sqrt{(2l'+1)(2l_1+1)(2l_2+1)}\, h^{(1)}_{l_1}(kr) j_{l_2}(ks_j) j_{l'}(ka_j) \begin{pmatrix} l_1 & l_2 & l' \\ 0 & 0 & 0\end{pmatrix} \\ &\times \begin{pmatrix} l_1 & l_2 & l' \\ m_1 & m'-m_1 & -m'\end{pmatrix} Y_{l_2,m'-m_1}(\hat{s}_j) Y_{l_1 m_1}(\hat{r}')\tilde{\mathbf{A}}^j_{lm,l'm'}\ . && (55)\end{aligned}$$

The calculation of $I^{\vec{r}}_\infty$ can be carried out in an analogous way as the determination of I^j_∞. In the calculation of $I^{\vec{r}}_j$ the integration is performed in the (j)-system, then the addition theorem (48) is used. This leads to Eq. (55).

One could insert the last results in Eq. (51) and drop the condition $kr' \gg 1$. This would yield an expression for the wave function valid for all r'. The only restriction to $\vec{r}\,'$ is that the addition theorem (48) of Hankel-functions has to hold. In order to determine the **S**-matrix it suffices to use $\vec{r}\,'$ far away from the scatterers, such that Eq. (4) becomes valid. Hence, inserting (51) in (4) we obtain

$$\mathbf{S}_{lm,l'm'} = \delta_{ll'}\delta_{mm'} - i\sum_{j'',l'',m''} \tilde{\mathbf{A}}^{j''}_{lm,l''m''}\tilde{\mathbf{D}}^{j''}_{l''m'',l'm'}\ . \tag{56}$$

We use $\tilde{\mathbf{A}}^j_{lm,l'm'} = \sum_{\tilde{m}=-l'}^{l'} \mathbf{A}^j_{lm,l'\tilde{m}} D^{l'}_{m'\tilde{m}}(j,gl)$ to get this result compatible with the results obtained in the first case. By this operation the N local coordinate systems appear and we obtain Eqs. (12) and (13).

B Symmetry Considerations

In order to simplify the determination of scattering resonances, given as the zeros of the determinant of the characteristic matrix **M**, the symmetry of the scattering configuration

can be used to block-diagonalize $\mathbf{M}$. (These operations are allowed as $\mathbf{M}-\mathbf{1}$ has been proven trace-class and as $\mathrm{Det}\,\mathbf{M}$ exists.) A similar approach was used in Ref. [37] in order to perform symmetry reductions in N-disk scattering systems in a semiclassical description.

The infinite square matrix $\mathbf{M}$ can be interpreted as a linear application acting on the square integrable functions defined on the surfaces of the N scatterers. In Sec. 2 we have seen that $\mathbf{M}$ contains the complete information on the geometry of the entire scattering system, so we have

$$[\mathbf{M}, \rho(g)] = 0 \; , \qquad \forall g \in G \; . \tag{57}$$

Here ρ denotes the linear representation of the symmetry group G acting in the same space as $\mathbf{M}$. As the entire scattering configuration can be constructed by successive applications of the symmetry transformations of G acting on an appropriate fundamental domain, the representation ρ is decomposable,

$$\rho = R \otimes \tilde{\rho} \; . \tag{58}$$

The representation R acts on the $|G|$ (= number of elements of G) copies of the fundamental domain and $\tilde{\rho}$ acts on an appropriate basis of the square integrable functions defined in the fundamental domain. Now it is easy to see that R is the regular representation [40] of G. If the symmetry group G is finite, the regular representation is, as is well known, reducible,

$$R = \bigoplus_c d_c D_c \; . \tag{59}$$

Here the index c runs over all conjugacy classes and D_c is the c-th irreducible representation of dimension d_c. Therefore, if we are dealing with scattering systems that possess only discrete symmetries (this suffices to ensure $|G| < \infty$ as we are dealing with finite, $N < \infty$, systems) we obtain

$$\mathrm{Det}\,\mathbf{M} = \prod_c (\mathrm{Det}\,\tilde{\mathbf{M}}_{D_c})^{d_c} \; . \tag{60}$$

The last result is inserted in Eq. (22) and formula (23) is obtained.

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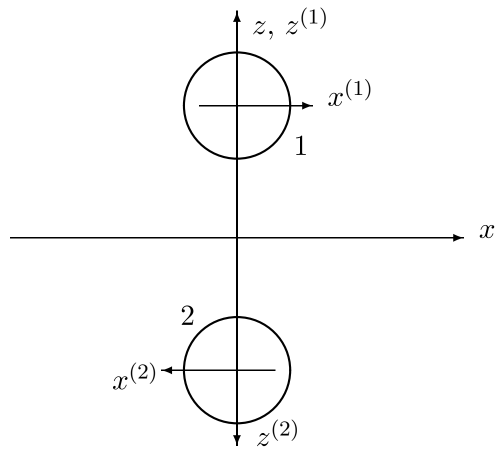

Figure 1: The two-sphere-configuration consisting of two equal spheres. The global and local coordinate systems used are also shown.

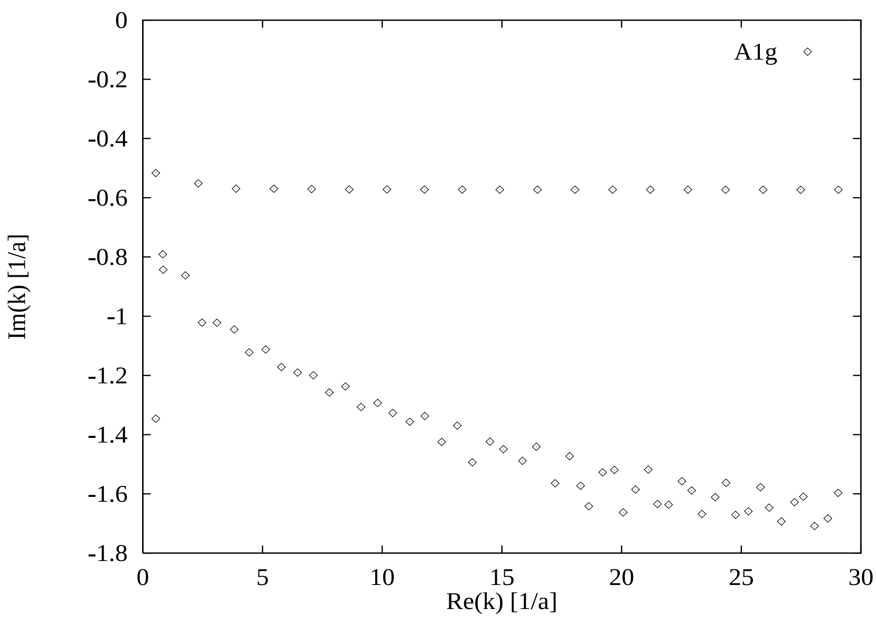

Figure 2: Quantum-mechanically calculated A_{1g}-resonances of the two-sphere system in the complex k-plane. The center-to-center seperation is $R = 6a$ and the wave number is measured in units of the inverse sphere radius a.

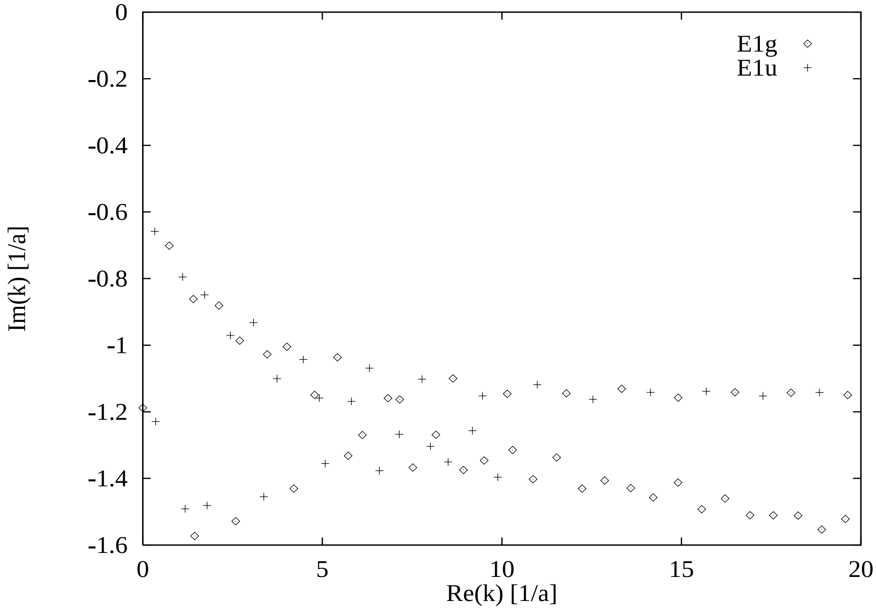

Figure 3: Quantum-mechanically calculated E_{1g}- and E_{1u}-resonances of the two-sphere system in the complex k-plane.

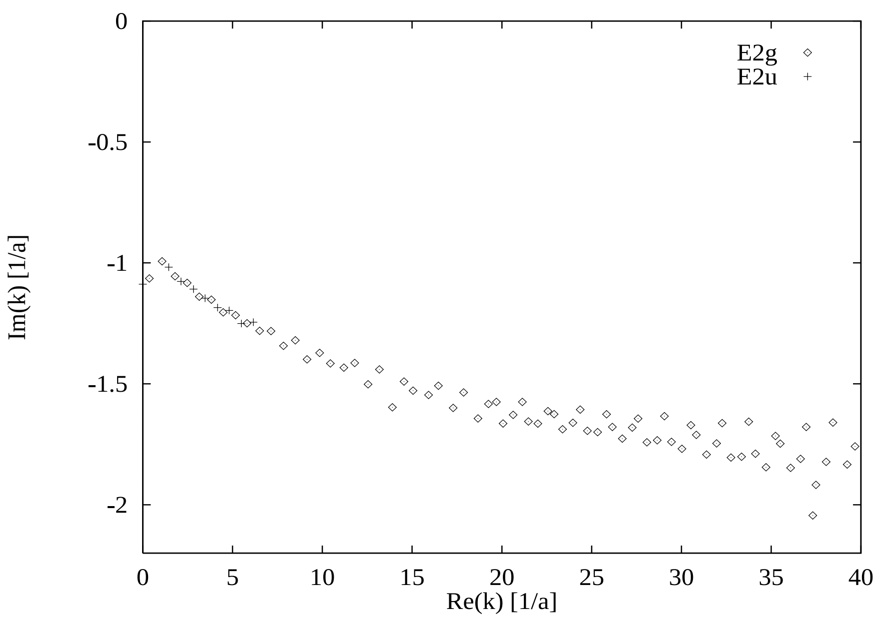

Figure 4: Quantum-mechanically calculated E_{2g}- and E_{2u}-resonances of the two-sphere system in the complex k-plane.

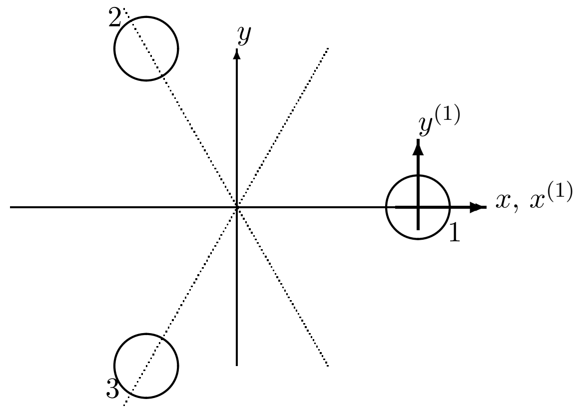

Figure 5: The three-sphere-configuration consisting of three equal spheres. The global and the local coordinate system of the first sphere are also shown. The remaining two local coordinate systems are obtained by rotations through $\frac{2\pi}{3}$ (sphere two) and $\frac{4\pi}{3}$ (sphere three) around the origin of the global system. All z-axes are perpendicular to the figure plane.

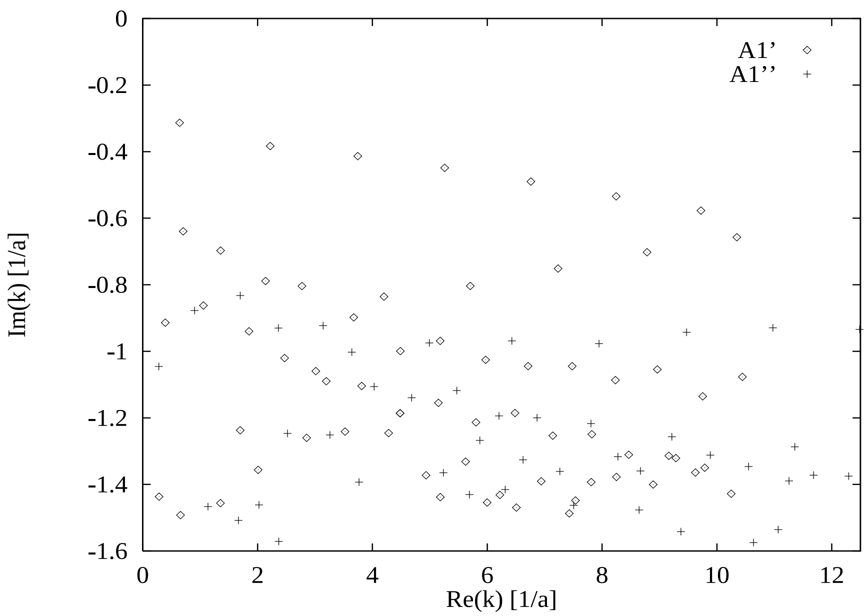

Figure 6: Quantum-mechanically calculated $A_1{}'$- and $A_1{}''$-resonances of the three-sphere-system in the complex k-plane.

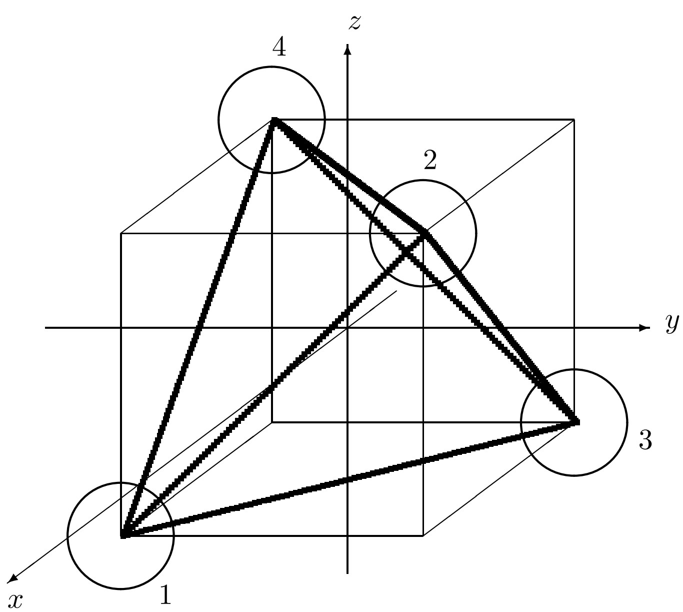

Figure 7: The four-sphere-configuration consists of four equal spheres at the corners of a regular tetrahedron (thick lines). In order to have a better visualization of the symmetries the tetrahedron is placed in a cube in whose center lies the origin of the global coordinate system (x, y, z).

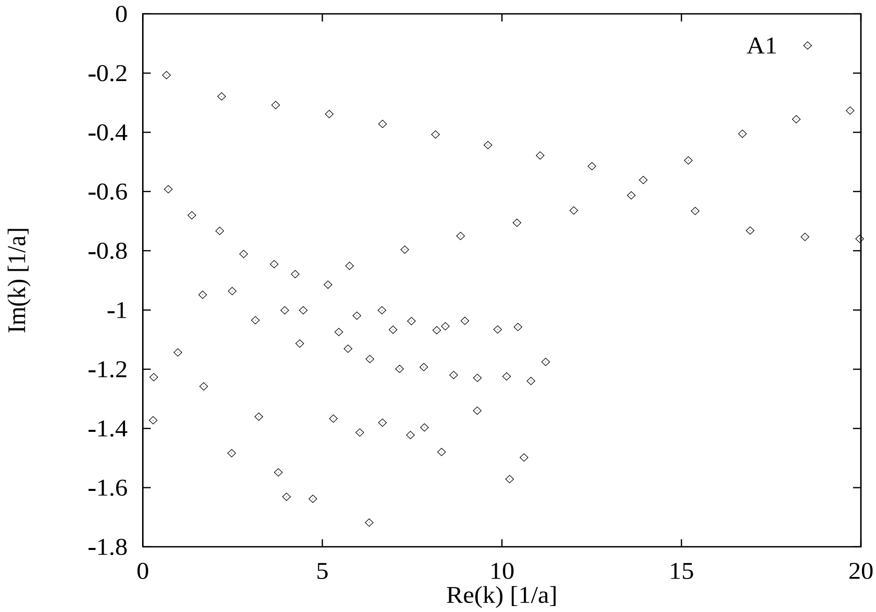

Figure 8: Quantum-mechanically calculated A_1-resonances of the four-sphere system in the complex k-plane. For numerical reasons only the first subleading resonances have been calculated.

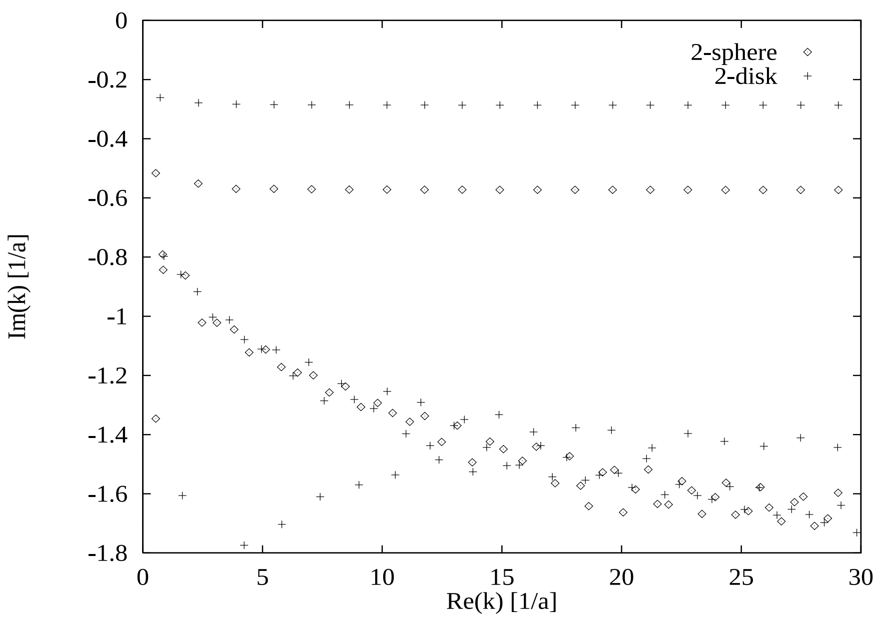

Figure 9: Comparison of the quantum-mechanically calculated resonances in the complex k-plane of the totally symmetric representations of the two-sphere and two-disk systems.

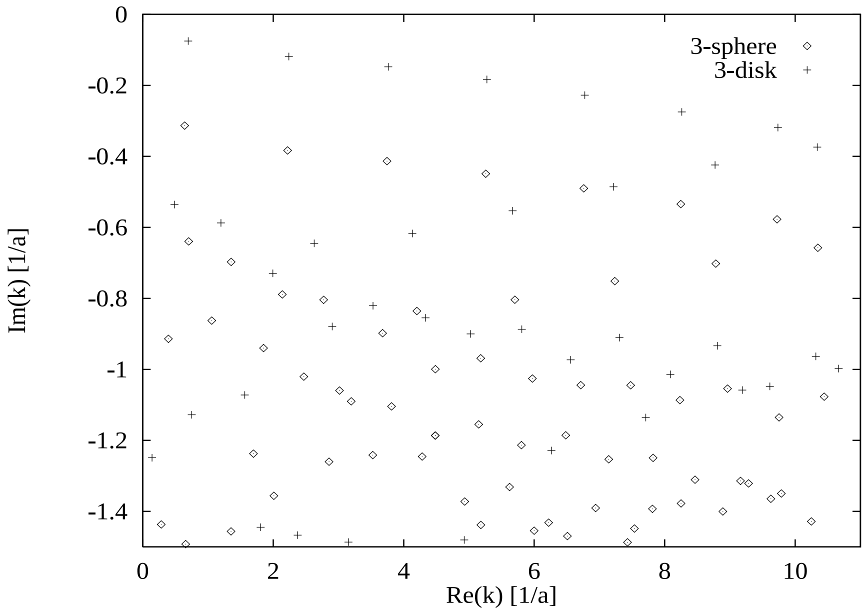

Figure 10: Comparison of the quantum-mechanically calculated resonances in the complex k-plane of the totally symmetric representations of the three-sphere and three-disk systems.

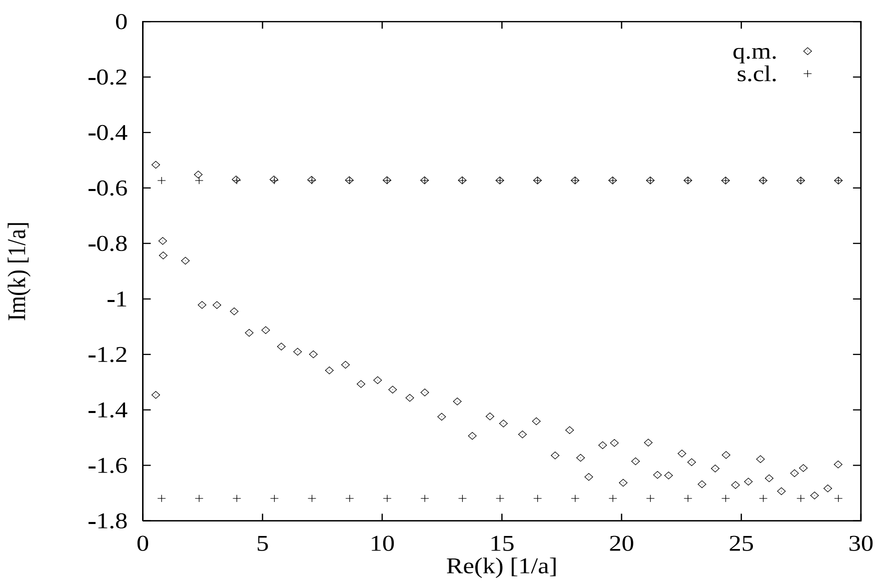

Figure 11: Comparison of quantum-mechanically (q.m.) and semiclassically (s.cl.) calculated resonances of the completely symmetric representation of the two-sphere system in the complex k-plane.